Separability criteria based on the Bloch representation of density matrices

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Abstract

We study the separability of bipartite quantum systems in arbitrary dimensions using the Bloch representation of their density matrix. This approach enables us to find an alternative characterization of the separability problem, from which we derive a necessary condition and sufficient conditions for separability. For a certain class of states the necessary condition and a sufficient condition turn out to be equivalent, therefore yielding a necessary and sufficient condition. The proofs of the sufficient conditions are constructive, thus providing decompositions in pure product states for the states that satisfy them. We provide examples that show the ability of these conditions to detect entanglement. In particular, the necessary condition is proved to be strong enough to detect bound entangled states.

1 Introduction

Let ρ denote the density operator, acting on the finite-dimensional Hilbert space $H = H_A \otimes H_B$, which describes the state of two quantum systems A and B. The state is said to be separable if ρ can be written as a convex combination of product vectors [1], i.e.

$$\rho = \sum_i p_i |\phi_i, \varphi_i\rangle\langle\phi_i, \varphi_i| = \sum_i p_i \, \rho_i^A \otimes \rho_i^B \, , \tag{1}$$

where $0 \leq p_i \leq 1$, $\sum_i p_i = 1$, and $|\phi_i, \varphi_i\rangle = |\phi_i\rangle_A \otimes |\varphi_i\rangle_B$ ($|\phi\rangle_A \in H_A$ and $|\varphi\rangle_B \in H_B$).

If ρ cannot be written as in Eq. (1), then the state is said to be entangled. Entanglement is responsible for many of the striking features of quantum theory and, therefore, it has been an object of special attention. Since the early years of quantum mechanics, it has been present in many of the debates regarding the foundations and implications of the theory (see e.g. [2]), but in the last ten years this interest has greatly increased, specially from a practical point of view, because entanglement is an essential ingredient in the applications of quantum

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information theory, such as quantum cryptography, dense coding, teleportation and quantum computation [3, 4]. As a consequence, much effort has been devoted to the so-called separability problem, which consists in finding mathematical conditions which provide a practical way to check whether a given state is entangled or not, since it is in general very hard to verify if a decomposition according to the definition of separability (1) exists. Up to now, a conclusive answer to the separability question can only be given when $\dim H_A = 2$ and $\dim H_B = 2$ or $\dim H_B = 3$, in which case the Peres-Horodecki criterion [5, 6] establishes that ρ is separable if and only if its partial transpose (i.e. transpose with respect to one of the subsystems) is positive. For higher dimensions this is just a necessary condition [6], since there exist entangled states with positive partial transpose (PPT) which are bound entangled (i.e. their entanglement cannot be distilled to the singlet form). Therefore the separability problem remains open. Much subsequent work has been devoted to finding necessary conditions for separability (see for example [7, 8, 9, 10, 11, 12, 13]), given that they can assure the presence of entanglement in experiments and that, in principle, they might complement the strong Peres-Horodecki criterion by detecting PPT entanglement. Nevertheless, there also exist a great variety of sufficient conditions (such as [14, 15]), non-operational necessary and sufficient conditions (see for instance [6, 16, 17]), or necessary and sufficient conditions which apply to restricted sets such as low-rank density matrices [18]. Furthermore, given a generic separable density matrix it is not known how to decompose it according to Eq. (1) save for the (2×2)-dimensional case [19, 20]. The (approximate) separability problem is NP-hard [21], but several authors have devised nontrivial algorithms for it (see [22] for a survey).

In this paper we derive a necessary condition and three sufficient conditions for the separability of bipartite quantum systems of arbitrary dimensions. The proofs of the latter conditions are constructive, so they provide decompositions in product states as in Eq. (1) for the separable states that fulfill them. Our results are obtained using the Bloch representation of density matrices, which has been used in previous works to characterize the separability of a certain class of bipartite qubit states [23] and to study the separability of bipartite states near the maximally mixed one [24, 25]. The approach presented here is different and more general. We will also provide examples that show the usefulness of the conditions derived here. Remarkably, the necessary condition is strong enough to detect PPT entangled states. Finally, we will compare this condition to the so-called computable cross-norm [9] or realignment [10] (CCNR) criterion, which exhibits a powerful PPT entanglement detection capability, showing that for a certain class of states our condition is stronger.

2 Bloch Representation

N-level quantum states are described by density operators, i.e. unit trace Hermitian positive semidefinite linear operators, which act on the Hilbert space $H \simeq \mathbb{C}^N$. The Hermitian operators acting on H constitute themselves a Hilbert space, the so-called Hilbert-Schmidt space $HS(H)$, with inner product $\langle \rho, \tau \rangle_{HS} = \mathrm{Tr}(\rho^\dagger \tau)$. Accordingly, the density operators can be expanded by any basis of this space. In particular, we can choose to expand ρ in terms of the identity operator I_N and the traceless Hermitian generators of $SU(N)$ λ_i

$(i = 1, 2, \ldots, N^2 - 1)$,

$$\rho = \frac{1}{N}(I_N + r_i \lambda_i), \tag{2}$$

where, as we shall do throughout this paper, we adhere to the convention of summation over repeated indices. The generators of $SU(N)$ satisfy the orthogonality relation

$$\langle \lambda_i, \lambda_j \rangle_{HS} = \mathrm{Tr}(\lambda_i \lambda_j) = 2\delta_{ij}, \tag{3}$$

and they are characterized by the structure constants of the corresponding Lie algebra, f_{ijk} and g_{ijk}, which are, respectively, completely antisymmetric and completely symmetric,

$$\lambda_i \lambda_j = \frac{2}{N}\delta_{ij} I_N + i f_{ijk}\lambda_k + g_{ijk}\lambda_k. \tag{4}$$

The generators can be easily constructed from any orthonormal basis $\{|a\rangle\}_{a=0}^{N-1}$ in H [26]. Let l, j, k be indices such that $0 \leq l \leq N-2$ and $0 \leq j < k \leq N-1$. Then, when $i = 1, \ldots, N-1$

$$\lambda_i = w_l \equiv \sqrt{\frac{2}{(l+1)(l+2)}} \left(\sum_{a=0}^{l} |a\rangle\langle a| - (l+1)|l+1\rangle\langle l+1| \right), \tag{5}$$

while when $i = N, \ldots, (N+2)(N-1)/2$

$$\lambda_i = u_{jk} \equiv |j\rangle\langle k| + |k\rangle\langle j|, \tag{6}$$

and when $i = N(N+1)/2, \ldots, N^2 - 1$

$$\lambda_i = v_{jk} \equiv -i(|j\rangle\langle k| - |k\rangle\langle j|). \tag{7}$$

The orthogonality relation (3) implies that the coefficients in (2) are given by

$$r_i = \frac{N}{2}\mathrm{Tr}(\rho\lambda_i). \tag{8}$$

Notice that the coefficient of I_N is fixed due to the unit trace condition. The vector $\mathbf{r} = (r_1 r_2 \cdots r_{N^2-1})^t \in \mathbb{R}^{N^2-1}$, which completely characterizes the density operator, is called Bloch vector or coherence vector. The representation (2) was introduced by Bloch [27] in the $N = 2$ case and generalized to arbitrary dimensions in [26]. It has an interesting appeal from the experimentalist point of view, since in this way it becomes clear how the density operator can be constructed from the expectation values of the operators λ_i,

$$\langle \lambda_i \rangle = \mathrm{Tr}(\rho\lambda_i) = \frac{2}{N} r_i. \tag{9}$$

As we have seen, every density operator admits a representation as in Eq. (2); however, the converse is not true. A matrix of the form (2) is of unit trace and Hermitian, but it might not be positive semidefinite, so to guarantee this property further restrictions must be added to the coherence vector. The set of all the Bloch vectors that constitute a density operator is known as the Bloch-vector space $B(\mathbb{R}^{N^2-1})$. It is widely known that in the case $N = 2$ this space equals the unit ball in $\mathbb{R}^3$ and pure states are represented by vectors on the

unit sphere. The problem of determining $B(\mathbb{R}^{N^2-1})$ when $N \geq 3$ is still open and a subject of current research (see for example [28] and references therein). However, many of its properties are known. For instance, using Eq. (4), one finds that for pure states ($\rho^2 = \rho$) it must hold

$$||\mathbf{r}||_2 = \sqrt{\frac{N(N-1)}{2}}, \quad r_i r_j g_{ijk} = (N-2) r_k, \tag{10}$$

where $||\cdot||_2$ is the Euclidean norm on $\mathbb{R}^{N^2-1}$.

In the case of mixed states, the conditions that the coherence vector must satisfy in order to represent a density operator have been recently provided in [29, 30]. Regrettably, their mathematical expression is rather cumbersome. It is also known [31, 32] that $B(\mathbb{R}^{N^2-1})$ is a subset of the ball $D_R(\mathbb{R}^{N^2-1})$ of radius $R = \sqrt{\frac{N(N-1)}{2}}$, which is the minimum ball containing it, and that the ball $D_r(\mathbb{R}^{N^2-1})$ of radius $r = \sqrt{\frac{N}{2(N-1)}}$ is included in $B(\mathbb{R}^{N^2-1})$. That is,

$$D_r(\mathbb{R}^{N^2-1}) \subseteq B(\mathbb{R}^{N^2-1}) \subseteq D_R(\mathbb{R}^{N^2-1}). \tag{11}$$

In the case of bipartite quantum systems of dimensions $M \times N$ ($H \simeq \mathbb{C}^M \otimes \mathbb{C}^N$) composed of subsystems A and B, we can analogously represent the density operators as[1]

$$\rho = \frac{1}{MN}(I_M \otimes I_N + r_i \lambda_i \otimes I_N + s_j I_M \otimes \tilde{\lambda}_j + t_{ij} \lambda_i \otimes \tilde{\lambda}_j), \tag{12}$$

where λ_i ($\tilde{\lambda}_j$) are the generators of $SU(M)$ ($SU(N)$). Notice that $\mathbf{r} \in \mathbb{R}^{M^2-1}$ and $\mathbf{s} \in \mathbb{R}^{N^2-1}$ are the coherence vectors of the subsystems, so that they can be determined locally,

$$\rho_A = \mathrm{Tr}_B \rho = \frac{1}{M}(I_M + r_i \lambda_i), \quad \rho_B = \mathrm{Tr}_A \rho = \frac{1}{N}(I_N + s_i \tilde{\lambda}_i). \tag{13}$$

The coefficients t_{ij}, responsible for the possible correlations, form the real matrix $T \in \mathbb{R}^{(M^2-1)\times(N^2-1)}$, and, as before, they can be easily obtained by

$$t_{ij} = \frac{MN}{4} \mathrm{Tr}(\rho \lambda_i \otimes \tilde{\lambda}_j) = \frac{MN}{4} \langle \lambda_i \otimes \tilde{\lambda}_j \rangle. \tag{14}$$

3 Separability Conditions from the Bloch Representation

The Bloch representation of bipartite quantum systems (12) allows us to find a simple characterization of separability for pure states.

Proposition 1: A pure bipartite quantum state with Bloch representation (12) is separable if and only if

$$T = \mathbf{r}\,\mathbf{s}^t \tag{15}$$

[1] This representation is sometimes referred in the literature as Fano form (see e. g. [33]), since this author was the first to consider it [34].

holds.

Proof: Simply notice that Eq. (12) can be rewritten as

$$\rho = \rho_A \otimes \rho_B + \frac{1}{MN}[(t_{ij} - r_i s_j)\lambda_i \otimes \tilde{\lambda}_j]. \tag{16}$$

Since the $\lambda_i \otimes \tilde{\lambda}_j$ are linearly independent, $(t_{ij} - r_i s_j)\lambda_i \otimes \tilde{\lambda}_j = 0$ if and only if $t_{ij} - r_i s_j = 0 \; \forall \, i, j$. $\square$

Remark 1: In the case of mixed states, Eq. (15) provides a sufficient condition for separability, since then $\rho = \rho_A \otimes \rho_B$.

Attending to Proposition 1, we can characterize separability from the Bloch representation point of view in the following terms:

A bipartite quantum state with Bloch representation (12) is separable if and only if there exist vectors $\mathbf{u}_i \in \mathbb{R}^{M^2-1}$ *and* $\mathbf{v}_i \in \mathbb{R}^{N^2-1}$ *satisfying Eq. (10) and weights* p_i *satisfying* $0 \leq p_i \leq 1$, $\sum_i p_i = 1$ *such that*

$$T = p_i \mathbf{u}_i \, \mathbf{v}_i^t, \quad \mathbf{r} = p_i \mathbf{u}_i, \quad \mathbf{s} = p_i \mathbf{v}_i \, . \tag{17}$$

This allows us to derive the two theorems below, which provide, respectively, a necessary condition and a sufficient condition for separability. We will make use of the Ky Fan norm $|| \cdot ||_{KF}$, which is commonly used in Matrix Analysis (the reader who is not familiarized with this issue can consult for example [35]). We recall that the singular value decomposition theorem ensures that every matrix $A \in \mathbb{C}^{m \times n}$ admits a factorization of the form $A = U \Sigma V^\dagger$ such that $\Sigma = (\sigma_{ij}) \in \mathbb{R}_+^{m \times n}$ with $\sigma_{ij} = 0$ whenever $i \neq j$, and $U \in \mathbb{C}^{m \times m}$, $V \in \mathbb{C}^{n \times n}$ are unitary matrices. The Ky Fan matrix norm is defined as the sum of the singular values $\sigma_i \equiv \sigma_{ii}$,

$$||A||_{KF} = \sum_{i=1}^{\min\{m,n\}} \sigma_i = \mathrm{Tr}\sqrt{A^\dagger A}. \tag{18}$$

This norm has previously been used in the context of the separability problem, though in a different way, in the CCNR criterion.

Theorem 1: If a bipartite state of $M \times N$ dimensions with Bloch representation (12) is separable, then

$$||T||_{KF} \leq \sqrt{\frac{MN(M-1)(N-1)}{4}} \tag{19}$$

must hold.

Proof: Since T has to admit a decomposition of the form (17) with

$$||\mathbf{u}_i||_2 = \sqrt{\frac{M(M-1)}{2}}, \quad ||\mathbf{v}_i||_2 = \sqrt{\frac{N(N-1)}{2}}, \tag{20}$$

we must have

$$||T||_{KF} \leq p_i ||\mathbf{u}_i \, \mathbf{v}_i^t||_{KF} = p_i \sqrt{\frac{MN(M-1)(N-1)}{4}} ||\mathbf{n}_i \, \tilde{\mathbf{n}}_i^t||_{KF}, \tag{21}$$

where $\mathbf{n}_i, \tilde{\mathbf{n}}_i$ are unit vectors. Thus, $||\mathbf{n}_i\, \tilde{\mathbf{n}}_i^t||_{KF} = 1\ \forall i$ and the result follows. $\square$

As said before, T contains all the information about the correlations, so that $||T||_{KF}$ measures in a certain sense the size of these correlations. In this way, Theorem 1 has a clear physical meaning: there is an upper bound to the correlations contained in a separable state. $||T||_{KF}$ is a consistent measure of the correlations since it is left invariant local changes of basis, i.e. it is invariant under local unitary transformations of the density operator. This fact was mentioned in [23] when $M = N = 2$; in the next proposition we give a general proof.

Proposition 2: Let U_A (U_B) denote a unitary transformation acting on subsystem A (B). If

$$\rho' = (U_A \otimes U_B)\rho \left(U_A^\dagger \otimes U_B^\dagger\right), \tag{22}$$

then $||T'||_{KF} = ||T||_{KF}$.

Proof: Let ρ_A and ρ'_A denote density operators acting on $H_A \simeq \mathbb{C}^M$ such that $\rho'_A = U_A \rho_A U_A^\dagger$. Since $||\cdot||_{HS}$ is unitarily invariant we have that $||\rho_A||_{HS} = ||\rho'_A||_{HS}$. But using the orthogonality relation (3) and Eq. (8) we find that

$$||\rho_A||_{HS}^2 = \frac{1}{M}\left(1 + \frac{2}{M}||\mathbf{r}||_2^2\right), \tag{23}$$

hence $||\mathbf{r}||_2 = ||\mathbf{r}'||_2$. This implies that the coherence vectors of different realizations of the same state are related by a rotation, i.e. there exists a rotation O_A acting on $\mathbb{R}^{M^2-1}$ such that $\mathbf{r}' = O_A\mathbf{r}$. This means that

$$U_A r_i \lambda_i U_A^\dagger = \left(O_A \mathbf{r}\right)_i \lambda_i. \tag{24}$$

Now, when a bipartite state ρ is subjected to a product unitary transformation (22) there will be rotations O_A acting on $\mathbb{R}^{M^2-1}$ and O_B acting on $\mathbb{R}^{N^2-1}$ such that

$$\mathbf{r}' = O_A\mathbf{r}, \quad \mathbf{s}' = O_B\mathbf{s}, \quad T' = O_A T O_B^\dagger. \tag{25}$$

Thus, the result follows taking into account that $||\cdot||_{KF}$ is unitarily invariant. $\square$

The characterization of the separability problem given in Eq. (17) suggests the possibility of obtaining a sufficient condition for separability using a constructive proof. One such condition is stated in the following proposition.

Proposition 3: If a bipartite state of $M \times N$ dimensions with Bloch representation (12) satisfies

$$\sqrt{\frac{2(M-1)}{M}}||\mathbf{r}||_2 + \sqrt{\frac{2(N-1)}{N}}||\mathbf{s}||_2 + \sqrt{\frac{4(M-1)(N-1)}{MN}}||T||_{KF} \leq 1, \tag{26}$$

then it is a separable state.

Proof: Let T have the singular value decomposition $T = \sigma_i \mathbf{u}_i\, \mathbf{v}_i^t$, with $||\mathbf{u}_i||_2 =$

$||\mathbf{v}_i||_2 = 1$. If we define

$$\widetilde{\mathbf{u}}_i = \sqrt{\frac{M}{2(M-1)}}\mathbf{u}_i, \quad \widetilde{\mathbf{v}}_i = \sqrt{\frac{N}{2(N-1)}}\mathbf{v}_i, \tag{27}$$

we can rewrite

$$T = \sqrt{\frac{4(M-1)(N-1)}{MN}}\sigma_i \widetilde{\mathbf{u}}_i\, \widetilde{\mathbf{v}}_i^t. \tag{28}$$

Then, if condition (26) holds, we can decompose ρ as the following convex combination of the density matrices ϱ_i, ϱ_i', ρ_r, ρ_s and $\frac{1}{MN}I_{MN}$,

$$\rho = \sqrt{\frac{4(M-1)(N-1)}{MN}}\frac{1}{2}\sigma_i(\varrho_i + \varrho_i') + \sqrt{\frac{2(M-1)}{M}}||\mathbf{r}||_2\rho_r + \sqrt{\frac{2(N-1)}{N}}||\mathbf{s}||_2\rho_s$$
$$+ \left(1 - \sqrt{\frac{2(M-1)}{M}}||\mathbf{r}||_2 - \sqrt{\frac{2(N-1)}{N}}||\mathbf{s}||_2 - \sqrt{\frac{4(M-1)(N-1)}{MN}}||T||_{KF}\right)\frac{I_{MN}}{MN}, \tag{29}$$

where ϱ_i, ϱ_i', ρ_r and ρ_s are such that

$$\mathbf{r}_i = \widetilde{\mathbf{u}}_i, \quad \mathbf{s}_i = \widetilde{\mathbf{v}}_i, \quad T_i = \widetilde{\mathbf{u}}_i\, \widetilde{\mathbf{v}}_i^t,$$

$$\mathbf{r}_i' = -\widetilde{\mathbf{u}}_i, \quad \mathbf{s}_i' = -\widetilde{\mathbf{v}}_i, \quad T_i' = \widetilde{\mathbf{u}}_i\, \widetilde{\mathbf{v}}_i^t,$$

$$\mathbf{r}_r = \sqrt{\frac{M}{2(M-1)}}\frac{\mathbf{r}}{||\mathbf{r}||_2}, \quad \mathbf{s}_r = 0, \quad T_r = 0,$$

$$\mathbf{r}_s = 0, \quad \mathbf{s}_s = \sqrt{\frac{N}{2(N-1)}}\frac{\mathbf{s}}{||\mathbf{s}||_2}, \quad T_s = 0.$$

Notice that by virtue of Eq. (11) all the above coherence vectors belong to the corresponding Bloch spaces and, therefore, the reductions of ϱ_i, ϱ_i', ρ_r and ρ_s constitute density matrices. Moreover, all these matrices satisfy condition (15), hence they are equal to the tensor product of their reductions. Therefore, they constitute density matrices and they are separable, and so must be ρ. □

One could ask whether Proposition 3 can be strengthened using a condition more involved than Eq. (26). As we shall see in the following theorem, the answer is positive.

Theorem 2: Let

$$c = \max\left\{\sqrt{\frac{2(M-1)}{M}}||\mathbf{r}||_2, \sqrt{\frac{2(N-1)}{N}}||\mathbf{s}||_2\right\}. \tag{30}$$

If a bipartite state of $M \times N$ dimensions with Bloch representation (12) such that $c \neq 0$ satisfies

$$c + \sqrt{\frac{4(M-1)(N-1)}{MN}}\left|\left|T - \frac{\mathbf{r}\,\mathbf{s}^t}{c}\right|\right|_{KF} \leq 1, \tag{31}$$

then it is a separable state.

Proof: On the analogy of the proof of Proposition 3, let $T - \frac{\mathbf{r}\,\mathbf{s}^t}{c}$ have the singular value decomposition $\sigma_i' \mathbf{x}_i\, \mathbf{y}_i^t$, where $||\mathbf{x}_i||_2 = ||\mathbf{y}_i||_2 = 1$. If we define

$$\widetilde{\mathbf{x}}_i = \sqrt{\frac{M}{2(M-1)}}\mathbf{x}_i, \quad \widetilde{\mathbf{y}}_i = \sqrt{\frac{N}{2(N-1)}}\mathbf{y}_i, \tag{32}$$

we can rewrite

$$T - \frac{\mathbf{r}\,\mathbf{s}^t}{c} = \sqrt{\frac{4(M-1)(N-1)}{MN}}\sigma_i' \widetilde{\mathbf{x}}_i\, \widetilde{\mathbf{y}}_i^t. \tag{33}$$

Now, if condition (31) holds we can decompose ρ in separable states as

$$\begin{aligned} \rho \quad &= \quad \sqrt{\frac{4(M-1)(N-1)}{MN}}\frac{1}{2}\sigma_i'(\varrho_i + \varrho_i') + c\rho_{rs} \\ &+ \quad \left(1 - c - \sqrt{\frac{4(M-1)(N-1)}{MN}}\left|\left|T - \frac{\mathbf{r}\,\mathbf{s}^t}{c}\right|\right|_{KF}\right)\frac{1}{MN}I_{MN}, \end{aligned} \tag{34}$$

where ϱ_i, ϱ_i' and ρ_{rs} are such that

$$\mathbf{r}_i = \widetilde{\mathbf{x}}_i, \quad \mathbf{s}_i = \widetilde{\mathbf{y}}_i, \quad T_i = \widetilde{\mathbf{x}}_i\, \widetilde{\mathbf{y}}_i^t,$$

$$\mathbf{r}_i' = -\widetilde{\mathbf{x}}_i, \quad \mathbf{s}_i' = -\widetilde{\mathbf{y}}_i, \quad T_i' = \widetilde{\mathbf{x}}_i\, \widetilde{\mathbf{y}}_i^t,$$

$$\mathbf{r}_{rs} = \frac{\mathbf{r}}{c}, \quad \mathbf{s}_{rs} = \frac{\mathbf{s}}{c}, \quad T_{rs} = \frac{\mathbf{r}\,\mathbf{s}^t}{c^2}.$$

As in the previous proof, and since

$$\frac{\mathbf{r}}{c} \leq \sqrt{\frac{M}{2(M-1)}}\frac{\mathbf{r}}{||\mathbf{r}||_2}, \quad \frac{\mathbf{s}}{c} \leq \sqrt{\frac{N}{2(N-1)}}\frac{\mathbf{s}}{||\mathbf{s}||_2},$$

all these coherence vectors belong to the corresponding Bloch spaces, and ϱ_i, ϱ_i' and ρ_{rs} satisfy (15). □

Notice that the use of the triangle inequality in Eq. (31) clearly shows that Theorem 2 is stronger than Proposition 3. Nevertheless, Proposition 3 provides the right way to understand the limit $c \to 0$ in Theorem 2. The proof of these two results is constructive, so for the states that fulfill Eqs. (26) and/or (31) they provide a decomposition in separable states. These states are in general not pure, but they are equal to the tensor product of their reductions, so to obtain a decomposition in product states as in Eq. (1) simply apply the spectral decomposition to the reductions of ϱ_i, ϱ_i', ρ_r, ρ_s and/or ρ_{rs}.

Remark 2: The conditions of Proposition 3 and Theorem 2 depend only on $\mathbf{r}$, $\mathbf{s}$ and T. However, there can also be obtained sufficient conditions for separability which include more parameters. For example, one can derive the following

sufficient condition, which also depends on the singular value decomposition of T,

$$\left\|\sqrt{\frac{N}{2(N-1)}}\mathbf{r}-\sigma_i\mathbf{u}_i\right\|_2+\left\|\sqrt{\frac{M}{2(M-1)}}\mathbf{s}-\sigma_i\mathbf{v}_i\right\|_2+||T||_{KF}\leq\sqrt{\frac{MN}{4(M-1)(N-1)}}, \tag{35}$$

since in this case ρ admits a decomposition in separable states as in Eq. (29) but with $\varrho_i'=\varrho_i$,

$$\mathbf{r}_r=\sqrt{\frac{M}{2(M-1)}}\frac{\mathbf{r}-\sqrt{\frac{2(N-1)}{N}}\sigma_i\mathbf{u}_i}{\left\|\mathbf{r}-\sqrt{\frac{2(N-1)}{N}}\sigma_i\mathbf{u}_i\right\|_2}\text{ and }\mathbf{s}_s=\sqrt{\frac{N}{2(N-1)}}\frac{\mathbf{s}-\sqrt{\frac{2(M-1)}{M}}\sigma_i\mathbf{v}_i}{\left\|\mathbf{s}-\sqrt{\frac{2(M-1)}{M}}\sigma_i\mathbf{v}_i\right\|_2}.$$

However, it seems reasonable to expect that condition (35) will be stronger than those of Proposition 3 and Theorem 2 in few cases.

For a restricted class of states the conditions of Theorem 1 and Proposition 3 take the same form, thus providing a necessary and sufficient condition which is equivalent to that of [23]:

Corollary 1: A bipartite state of qubits ($M=N=2$) with maximally mixed subsystems (i.e. $\mathbf{r}=\mathbf{s}=0$) is separable if and only if $||T||_{KF}\leq 1$.

4 Efficacy of the New Criteria

4.1 Examples

In what follows we provide examples of the usefulness of the criteria derived in the previous section to detect entanglement. We start by showing that Theorem 1 is strong enough to detect bound entanglement.

Example 1: Consider the following 3×3 PPT entangled state found in [36]:

$$\rho=\frac{1}{4}\left(I_9-\sum_{i=0}^{4}|\psi_i\rangle\langle\psi_i|\right), \tag{36}$$

where $|\psi_0\rangle=|0\rangle(|0\rangle-|1\rangle)/\sqrt{2}$, $|\psi_1\rangle=(|0\rangle-|1\rangle)|2\rangle/\sqrt{2}$, $|\psi_2\rangle=|2\rangle(|1\rangle-|2\rangle)/\sqrt{2}$, $|\psi_3\rangle=(|1\rangle-|2\rangle)|0\rangle/\sqrt{2}$ and $|\psi_4\rangle=(|0\rangle+|1\rangle+|2\rangle)(|0\rangle+|1\rangle+|2\rangle)/3$. To construct the Bloch representation of this state we use as generators of $SU(3)$ the Gell-Mann operators, which are a reordering of those of Eqs. (5)-(7),

$$\lambda_1=u_{01},\ \lambda_2=v_{01},\ \lambda_3=w_0,\ \lambda_4=u_{02},\ \lambda_5=v_{02},\ \lambda_6=u_{12},\ \lambda_7=v_{12},\ \lambda_8=w_1. \tag{37}$$

Then, for the state (36) one readily finds

$$T = -\frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 0 & \frac{\sqrt{27}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{9}{4} & 0 & -\frac{9}{8} & 0 & 0 & 0 & 0 & \frac{\sqrt{27}}{8} \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -\frac{9}{4} & 1 & 0 & 1 & 0 & -\frac{\sqrt{27}}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{27}}{4} & 0 & \frac{\sqrt{27}}{8} & 0 & 0 & \frac{\sqrt{27}}{2} & 0 & -\frac{3}{8} \end{pmatrix}, \tag{38}$$

so that $||T||_{KF} \simeq 3.1603$, which violates condition (19). Thus, using Theorem 1 we know that the state is entangled.

The above example proves that there exist cases in which Theorem 1 is stronger than the PPT criterion. One can see that this is not true in general, not even for the 2×2 case.

Example 2: Consider the following bipartite qubit state,

$$\rho_{\pm} = p|\psi^{\pm}\rangle\langle\psi^{\pm}| + (1-p)|00\rangle\langle 00|\,, \tag{39}$$

where $p \in [0,1]$ and

$$|\psi^{\pm}\rangle = \frac{1}{\sqrt{2}}\big(|01\rangle \pm |10\rangle\big). \tag{40}$$

The Peres-Horodecki criterion establishes that state (39) is separable iff $p = 0$ [5]. For its Bloch representation we use as generators of $SU(2)$ the standard Pauli matrices $\sigma_x = u_{01}$, $\sigma_y = v_{01}$ and $\sigma_z = w_0$, thus finding that

$$\rho_{\pm} = \frac{1}{4}(I_2 \otimes I_2 + (1-p)\sigma_z \otimes I_2 + (1-p) I_2 \otimes \sigma_z \pm p\,\sigma_x \otimes \sigma_x \pm p\,\sigma_y \otimes \sigma_y + (1-2p)\sigma_z \otimes \sigma_z). \tag{41}$$

Therefore, $||T||_{KF} = 2p + |1-2p|$, which implies that $||T||_{KF} \leq 1$ if $p \leq 1/2$, so entanglement is detected only if $p > 1/2$.

Example 3: Werner states [1] in arbitrary dimensions ($M = N = D$) are those whose density matrices are invariant under transformations of the form $\big(U \otimes U\big)\rho\left(U^{\dagger} \otimes U^{\dagger}\right)$. They can be written as

$$\rho_W = \frac{1}{D^3 - D}[(D-\phi) I_D \otimes I_D + (D\phi - 1)V], \tag{42}$$

where $-1 \leq \phi \leq 1$ and V is the "flip" or "swap" operator defined by $V\varphi \otimes \widetilde{\varphi} = \widetilde{\varphi} \otimes \varphi$. These states are separable iff $\phi \geq 0$ [1]. Using Eq. (14) or inverting Eqs. (5)-(7) we find that

$$V = \sum_{i,j} |ij\rangle\langle ji| = \frac{1}{D} I_D \otimes I_D + \frac{1}{2}\sum_{l} w_l \otimes w_l + \frac{1}{2}\sum_{j<k}(u_{jk} \otimes u_{jk} + v_{jk} \otimes v_{jk}), \tag{43}$$

so that

$$\rho_W = \frac{1}{D^2}\left(I_D \otimes I_D + \frac{D(D\phi - 1)}{2(D^2-1)}\lambda_i \otimes \lambda_i\right), \tag{44}$$

where λ_i are the generators of $SU(D)$ defined as in Eqs. (5)-(7). Then, $||T||_{KF} = D|D\phi - 1|/2$, so that Theorem 1 only recognizes entanglement when $\phi \leq (2-D)/D$, while Proposition 3 guarantees that the state is separable if $(D-2)/[D(D-1)] \leq \phi \leq 1/(D-1)$. When the latter condition holds, we can provide the decomposition in product states. To illustrate the procedure, consider the Werner state in, for simplicity, 2×2 dimensions. In this case $V = I_2 \otimes I_2 - 2|\psi^-\rangle\langle\psi^-|$, and defining $p = (1-2\phi)/3$ the state takes the simple form

$$\rho = \frac{1-p}{4} I_2 \otimes I_2 + p|\psi^-\rangle\langle\psi^-| = \frac{1}{4}(I_2 \otimes I_2 - p\,\sigma_x \otimes \sigma_x - p\,\sigma_y \otimes \sigma_y - p\,\sigma_z \otimes \sigma_z). \quad (45)$$

From Corollary 1 we obtain that ρ is separable iff $p \leq 1/3$ as expected. From Proposition 3 we find that

$$\rho = \sum_{i=x,y,z} \sum_{j=1}^{2} \frac{p}{2} \rho_j^{(i)} + (1-3p)\frac{1}{4}(I_2 \otimes I_2), \quad (46)$$

where

$$\rho_1^{(i)} = \frac{1}{4}(I_2 \otimes I_2 + \sigma_i \otimes I_2 - I_2 \otimes \sigma_i - \sigma_i \otimes \sigma_i), \quad \rho_2^{(i)} = \frac{1}{4}(I_2 \otimes I_2 - \sigma_i \otimes I_2 + I_2 \otimes \sigma_i - \sigma_i \otimes \sigma_i). \quad (47)$$

In this case we can reduce the number of product states in the decomposition to 8 by noticing that $\rho_1^{(i)} = |01\rangle_i\langle 01|$ and $\rho_2^{(i)} = |10\rangle_i\langle 10|$, where $\{|0\rangle_i, |1\rangle_i\}$ denote the eigenvectors of σ_i, so that, for instance,

$$\begin{aligned} \rho = &\sum_{i=x,y} \frac{p}{2}(|01\rangle_i\langle 01| + |10\rangle_i\langle 10|) + \frac{1-p}{4}(|01\rangle_z\langle 01| + |10\rangle_z\langle 10|) + \\ &+ \frac{1-3p}{4}(|00\rangle_z\langle 00| + |11\rangle_z\langle 11|). \end{aligned} \quad (48)$$

It is known, however, that a separable bipartite qubit state admits a decomposition in a number of product states less than or equal to 4 [19, 20].

Example 4: Isotropic states [7] in arbitrary dimensions ($M = N = D$) are invariant under transformations of the form $(U \otimes U^*)\rho\,(U^\dagger \otimes U^{*\dagger})$. They can be written as mixtures of the maximally mixed state and the maximally entangled state

$$|\Psi\rangle = \frac{1}{\sqrt{D}} \sum_{a=0}^{D-1} |aa\rangle, \quad (49)$$

so they read[2]

$$\rho = \frac{1-p}{D^2} I_D \otimes I_D + p|\Psi\rangle\langle\Psi|. \quad (50)$$

These states are known to be separable iff $p \leq (D+1)^{-1}$ [7] (see also [25, 37]). Their Bloch representation can be easily found as in the Werner case, and it is

[2] In the two-qubit case the Werner ($U \otimes U$ invariant) states (45) and isotropic ($U \otimes U^*$ invariant) states (50) are identical up to a local unitary transformation. For this reason some authors refer to the isotropic states as generalized Werner states, which might lead to confusion.

given by

$$\rho = \frac{1}{D^2}\left(I_D \otimes I_D + \frac{pD}{2}\sum_{i=1}^{(D+2)(D-1)/2} \lambda_i \otimes \lambda_i - \frac{pD}{2}\sum_{i=D(D+1)/2}^{D^2-1} \lambda_i \otimes \lambda_i\right), \tag{51}$$

where, as before, λ_i are the generators of $SU(D)$ defined in Eqs. (5)-(7). Now, $||T||_{KF} = pD(D^2-1)/2$. Thus, Theorem 1 is strong enough to detect all the entangled states ($||T||_{KF} \leq D(D-1)/2 \Leftrightarrow p \leq (D+1)^{-1}$), while Proposition 3 ensures that the states are separable when $p \leq (D+1)^{-1}(D-1)^{-2}$.

4.2 Comparison with the CCNR criterion

Let ρ be written in terms of the canonical basis $\{E_{ij} \otimes E_{kl}\}$ of $HS(H_A \otimes H_B)$ as

$$\rho = c_{ijkl} E_{ij} \otimes E_{kl}. \tag{52}$$

The computable cross-norm criterion, proposed by O. Rudolph (see [9, 38] and references therein), states that for all separable states the operator $U(\rho)$ acting on $HS(H_A \otimes H_B)$ defined by

$$U(\rho) \equiv c_{ijkl}|E_{ij}\rangle\langle E_{kl}|, \tag{53}$$

where $|E_{mn}\rangle$ denotes the ket vector with respect to the inner product in $HS(H_A)$ or $HS(H_B)$, is such that $||U(\rho)||_{KF} \leq 1$. Soon after, K. Chen and L.-A. Wu derived the realignment method [10], which yields the same results as the cross-norm criterion from simple matrix analysis. Basically, it states that a certain realigned version of a separable density matrix cannot have Ky Fan norm greater than one, thus providing a simple way to compute this condition. This is why we refer to it as the CCNR criterion. Like Theorem 1, it is able to detect all entangled isotropic states and recognizes entanglement for the same range of Werner states [9]. Although being weaker than the PPT criterion in 2×2 dimensions, it is also capable of detecting bound entangled states. However, the CCNR criterion detects optimally the entanglement of the state of Example 2 [9], so one could think that it is stronger than Theorem 1. To check this possibility and to evaluate the ability of bound entanglement detection of Theorem 1, we have programmed a routine that generates 10^6 random 3×3 PPT entangled states following [39]. Our theorem detected entanglement in about 4% of the states while the CCNR criterion recognized 18% of the states as entangled. Moreover, every state detected by Theorem 1 was also detected by the CCNR criterion. This suggests that the CCNR criterion is stronger than Theorem 1 when $M = N$. We will show that this is indeed the case, but we will also see that this is not true when $M \neq N$. First we will prove the following lemma:

Lemma 1:

$$\left|\left|\begin{pmatrix} A & B \\ C & D \end{pmatrix}\right|\right|_{KF} \geq ||A||_{KF} + ||D||_{KF},$$

where A, B, C, D are complex matrices of adequate dimensions.

Proof: Let A and D have the singular value decompositions $A = U_A \Sigma_A V_A^\dagger$ and $D = U_D \Sigma_D V_D^\dagger$. It is clear from the definition that the Ky Fan norm is unitarily

invariant. Therefore, we have that

$$\left|\left|\begin{pmatrix} A & B \\ C & D \end{pmatrix}\right|\right|_{KF} = \left|\left|\begin{pmatrix} U_A^\dagger & 0 \\ 0 & U_D^\dagger \end{pmatrix}\begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} V_A & 0 \\ 0 & V_D \end{pmatrix}\right|\right|_{KF}$$
$$\geq \text{Tr } \Sigma_A + \text{Tr } \Sigma_D, \tag{54}$$

where we have used that $||X||_{KF} \geq \text{Tr } X$, which is a direct consequence of the following characterization of the Ky Fan norm (see Eq. (3.4.7) in [35]):

$$||X||_{KF} = \max\{|\text{Tr } XU| : U \text{ is unitary}\}. \tag{55}$$

□

Proposition 4: In the case of states with maximally mixed subsystems Theorem 1 is stronger than the CCNR criterion when $M \neq N$, while when $M = N$ they are equivalent.

Proof: When $\mathbf{r} = \mathbf{s} = 0$ we have that

$$U(\rho) = \frac{1}{MN}(|I_M\rangle\langle I_N| + t_{ij}|\lambda_i\rangle\langle\tilde{\lambda}_j|). \tag{56}$$

Since the matrix associated to the operator $U(\rho)$ is in this case block-diagonal we find that

$$||U(\rho)||_{KF} = \frac{1}{\sqrt{MN}}\left|\left|\frac{|I_M\rangle}{\sqrt{M}}\frac{\langle I_N|}{\sqrt{N}}\right|\right|_{KF} + \frac{2}{MN}\left|\left|t_{ij}\frac{|\lambda_i\rangle}{\sqrt{2}}\frac{\langle\tilde{\lambda}_j|}{\sqrt{2}}\right|\right|_{KF}$$
$$= \frac{1}{\sqrt{MN}} + \frac{2}{MN}||T||_{KF}. \tag{57}$$

Thus, for states with maximally mixed subsystems the CCNR criterion is equivalent to

$$||T||_{KF} \leq \frac{\sqrt{MN}(\sqrt{MN}-1)}{2}, \tag{58}$$

from which the statement readily follows. □

Proposition 5: The CCNR criterion is stronger than Theorem 1 when $M = N$.

Proof: Since in this case in general $\mathbf{r}, \mathbf{s} \neq 0$, the matrix associated to the operator $U(\rho)$ is no longer block-diagonal. Hence, using Lemma 1, we now have that

$$||U(\rho)||_{KF} \geq \frac{1}{N} + \frac{2}{N^2}||T||_{KF}, \tag{59}$$

which proves the result considering that in the $M = N$ case the condition of Theorem 1 can be written as

$$\frac{1}{N} + \frac{2}{N^2}||T||_{KF} \leq 1. \tag{60}$$

□

Proposition 4 explains why both criteria yield the same results for Werner and isotropic states. However, since T is diagonal in these cases, the computations are much simpler in our formalism than in that of the CCNR criterion.

Furthermore, when $M \neq N$ we have explicitly constructed entangled states which are detected by Theorem 1 but not by the CCNR criterion. Regrettably, Theorem 1 is not able to detect the PPT entangled states in 2×4 dimensions constructed by P. Horodecki in [40].

5 Summary and Conclusions

We have used the Bloch representation of density matrices of bipartite quantum systems in arbitrary dimensions $M \times N$, which relies on two coherence vectors $\mathbf{r} \in \mathbb{R}^{M^2-1}$, $\mathbf{s} \in \mathbb{R}^{N^2-1}$ and a correlation matrix $T \in \mathbb{R}^{(M^2-1)\times(N^2-1)}$, to study their separability. This approach has led to an alternative formulation of the separability problem, which has allowed us to characterize entangled pure states (Proposition 1), and to derive a necessary condition (Theorem 1) and three sufficient conditions (Proposition 3, Theorem 2 and Remark 2) for the separability of general states. In the case of bipartite systems of qubits with maximally mixed subsystems Theorem 1 and Proposition 3 take the same form, thus yielding a necessary and sufficient condition for separability. We have shown that, despite being weaker than the PPT criterion in 2×2 dimensions, Theorem 1 is strong enough to detect PPT entangled states. We have also shown that it is capable of recognizing all entangled isotropic states in arbitrary dimensions but not all Werner states, like the CCNR criterion. Although the CCNR criterion turns out to be stronger than Theorem 1 when $M = N$, we have also proved that our theorem is stronger than the CCNR criterion for states with maximally disordered subsystems when $M \neq N$. Therefore, although Theorem 1 does not fully characterize separability, we believe that in combination with the above criteria it can improve our ability to understand and detect entanglement. Theorem 2, together with Proposition 3 (which is weaker save for the limiting case $c = 0$) and the result of Remark 2 (which is more involved), offers a sufficiency test of separability, which, as a by-product, provides a decomposition in product states of the states that satisfy its hypothesis. $||T||_{KF}$ acts as a measure of the correlations inside a bipartite state and it is left invariant under local unitary transformations of the density matrix. This suggests the possibility of considering it as a rough measure of entanglement, as in the case of the realignment method [10]. We think that this subject deserves further study. We also believe that a deeper understanding of the geometrical character of the Bloch-vector space could lead to an improvement of the separability conditions presented here.

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